Numerical Simulation of Reactive Flow

SECOND EDITION

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An Overview of Numerical Simulation

Reactive flows include a broad range of phenomena, such as flames, detonations, chemical lasers, the earth's atmosphere, stars and supernovae, and perhaps even the elementary particle interactions in the very early stages of the universe. There are striking physical differences among these flows, even though the general forms of the underlying equations are all quite similar. Therefore, considerations and procedures for constructing numerical models of these systems are also similar. The obvious and major differences are in the scales of the phenomena, the input data, the mathematical approximations that arise in representing different contributing physical processes, and the strength of the coupling among these processes.

For example, in flames and detonations, there is a close coupling among the chemical reactions, subsequent heat release, and the fluid dynamics, so that all of the processes must be considered simultaneously. In the earth's upper atmosphere, which is a weakly ionized plasma in a background neutral wind, the chemical reactions among ionized gases and the fluid dynamics are weakly coupled. These reactions take place in the background provided by the neutral gas motions. The sun's atmosphere is highly ionized, with reactions among photons, electrons, and ionized and neutral atomic species, all in the presence of strong electromagnetic fields. A Type Ia supernova creates the heavier elements in the periodic table through a series of strongly coupled thermonuclear reactions that occur in nuclear flames and detonations. The types of reactions, the major physical processes, and the degree and type of coupling among the processes vary substantially in these systems. Sometimes reactions are essentially decoupled from the fluid flow, sometimes radiation is important, and sometimes diffusive transport effects are important. These very different systems, however, are generally all dynamic and unsteady.

1–1. Some Comments on Terminology

The words *model*, *simulation*, *algorithm*, *numerical*, and *computational* are used repeatedly in this book. Even though these words seem easy enough to understand and use in ordinary conversation, their technical use is confused and imprecise. To different individuals and research communities, these words have different and sometimes overlapping meanings. To attack this technical "Tower of Babel" by proposing rigid definitions would

only add more confusion. Here, instead, we discuss some of the nuances of key terms used in this book, and then try to use the terms consistently.

What is generally meant by modeling is much broader than what is generally meant by simulation. A simulation attempts to imitate the dynamic behavior of a system and to predict the sequence of events that control that behavior. Modeling is generally used in a broader, more static sense: a model can represent a dynamic phenomenon in its entirety without specifying its evolution. A model can be a formula, a quantitative relation, a collection of empirical data, a set of equations, or even its equivalent analog circuit.

The objective of modeling is not necessarily to produce an exact copy of a system, but to reproduce certain salient features of the system. Because approximations are made to derive the model, it is understood that the model is an imperfect representation of the system. The result is that a model is invalid in some regimes and imprecise by some amount almost everywhere. A simulation, then, exercises a model or collection of models for a particular choice of physical parameters, initial conditions, and boundary conditions.

Throughout the literature, however, the use of the terms *modeling* and *simulation* overlap, and they are sometimes used interchangeably. The use of the words modeling and simulation has been further confused recently because several communities have adapted the terms to mean the use of very fast, data-driven models to create a virtual reality for interactive training or planning purposes. To combat the confusion caused by this degraded use of the terms, we usually hear the modified descriptions "detailed simulation," "detailed modeling," "high-fidelity simulation," or "fundamental model" to mean the careful scientific and engineering computations that are the subject of this book.

The terms *numerical* and *computational* are often used interchangeably, although they have somewhat different meanings. Numerical analysis, generally a theoretical subject whose main practical application is to solve problems on computers, is not all computational. Computational work in simulations is not all numerical. For example, a reactive-flow computation may involve interactive systems programming, text manipulation, data management, graphics, and so on. Here we consider models and algorithms as computational when they describe how the problem is broken down, represented, manipulated, and stored in the computer. We use the word *numerical* to describe techniques, methods, and algorithms when they concern the calculation of numbers or the quantitative evaluation of formulas and equations.

An *algorithm* is a solution procedure used to implement a model. It is not a model, and it is not necessarily numerical. Not every model has an algorithm associated with it; there simply might not be an algorithm to implement a model. A numerical simulation does not necessarily solve the equations that make up the mathematical model directly. The words *advance* and *integrate* might be more appropriate within the context of a simulation than the word *solve*. As the general reactive-flow problem varies in time, we solve a set of time-dependent, reactive Navier-Stokes equations that have been converted into a set of discretized algebraic equations in the computational model to advance the overall mathematical model. This algebraic set of equations is derived from the original set of partial differential equations in the mathematical model. Algorithms are substituted for the various mathematical terms, for their interactions, and thus for the underlying physical phenomena.

1–2. A Classification of Models

One useful classification of models distinguishes among three levels: fundamental, phenomenological, and empirical. In this sequence of levels, the models are increasingly coarse and are solved correspondingly faster. Making appropriate choices for the level of models to use can produce very practical composite reactive-flow models for solving difficult problems.

A *fundamental model*, often called a *detailed model*, describes the properties or behavior of a system starting with as many basic physical assumptions, or *first principles*, as possible. The problems that such a model can treat are limited in scope because of the expense and complexity of the calculation. Thus the usual objective is to simulate one isolated type of process or interaction. Such models can, however, be extremely detailed and exact in what they do cover. What should be a fundamental or detailed model in a reactive-flow simulation is problem dependent. It is defined by what is currently possible to do for that problem, or what is actually needed to represent the behavior of the system being simulated.

Detailed models can provide constants or other information for use in more general but less rigorous calculations. For example, quantum mechanical calculations of the potential energy surface of a molecule often provide information on the chemical reaction pathways and reaction rates used in more phenomenological continuum representations of reacting fluids. The continuum model itself may be made up of submodels that themselves may be fundamental, phenomenological, or empirical. An important objective of detailed modeling is to develop computational models with well-understood ranges of validity and accuracy. In principle, the broader the range of validity, the more generally useful the model is and the more expensive it is to use.

Phenomenological models and *empirical models* must be used when the time or space scales of the physical processes are too disparate to resolve consistently in one calculation. Macroscopic, averaged models of the small-scale processes become the phenomenological models that appear in the governing equations. For example, in the detailed models of flames considered later in this book, the chemical rate constants, diffusive transport coefficients, and equations of state cannot be determined simultaneously with the convective flow. These three types of models represent atomic-scale processes that have been averaged over assumed Maxwellian distributions of particles to derive the continuous, fluid description. These quantities are phenomenologies representing processes that occur on a scale too small to be resolved in a detailed way in the fluid computation itself.

Often the exact mathematical forms of terms in the governing equations are not known. Alternatively, these terms, though known, may be too complex to evaluate. In these cases, a simpler, approximate form must be used. This approximate *phenomenological* form is usually motivated by physical considerations and contains input data obtained from fits to experimental data or more fundamental theories or simulations. Often global constraints and conservation conditions are used to derive the phenomenological model. Turbulence models are examples of phenomenologies in which complex interactions are modeled by equations with physically reasonable forms. These models are then calibrated by adjusting coefficients to fit data derived from experiments or from more specialized, detailed simulations. Other examples include an energy release model for a chemical system, and a

parametric model for soot formation. A phenomenological model is based on a formula or algorithm that represents our intuitive, qualitative understanding of a particular physical situation. Thus, it must be calibrated with a more basic theory or an experiment. Over time these phenomenologies often acquire the reputation of a fundamental model without the corresponding reliability or accuracy. The Arrhenius reaction rate formula for chemical reactions is a good example of this.

Empirical models are either direct fits of data to a given mathematical formula or are data used directly in tabular form. Because the data are usually derived from experiments, they include extraneous effects, such as measurement interference or equipment calibration errors. A caveat attending such models is that they can only be used for interpolation, not extrapolation. This is true with respect to both the physical parameter range over which the model is valid and the particular physical environment in which it is used. Chemical rate constants are usually empirical models. Other examples of empirical models are tables of the rate at which smoke diffuses through a chamber, the rate a fire spreads through a building, or the rate of chemical energy release in a turbulent flame.

In this book we are interested in numerical simulations of reactive flows in which fluid dynamics, chemistry, and a variety of diffusive transport processes play important, dynamic, and interacting roles. For example, consider a propagating laminar flame, for which we construct a detailed model that solves the compressible Navier-Stokes equations with chemical reactions. The fluid dynamics may be solved by a very accurate numerical method and can be considered a fundamental model of convective transport. The chemical reaction rate coefficients are either phenomenological models if they are taken from fundamental calculations that have been fit into an analytic form, or empirical models if they are fits to experimental data. The equation of state may be a table compiled from experiments. Diffusion constants could be estimates based on intelligent guesses, or they could come from experiments or theoretical studies. This detailed model of a flame would become more phenomenological and less detailed if the set of chemical rate equations were replaced by a simplified "reduced" set of equations, or if the radiative effects were approximated by a single loss term instead of solving the equations of radiative transport.

1–3. Statistical Averaging or Chunking

The reactive Navier-Stokes equations that we use to describe a flame do not solve for the behavior of individual particles. They assume that the medium is a continuous, macroscopic fluid. This continuum approximation incorporates statistical averaging processes performed over the small-scale particle dynamics that we know are present.

The process in which the small-scale phenomena are averaged to produce a global quantity or interaction law has been called *chunking*, which means that microscopic complexity becomes statistically simplified, or chunked at a macroscopic level (Hofstadter 1979). Chunking reduces the number of degrees of freedom needed to describe the behavior of a system. The chunked behavior of a system follows relatively simple laws that approximate the statistical behavior of the microscopically complicated physical system. For example, complete, detailed knowledge of quarks and chromodynamics is not necessary for understanding many aspects of the composition and dynamics of atoms and nuclei. The

detailed interactions of every individual molecule in a system are not needed to explain a propagating laminar flame.

As we concentrate attention on more macroscopic scales and interactions, further chunking is needed to obtain usable models. Nuclear physics, for all but extremely high-energy collisions, chunks the behavior of subelementary particles to create protons and neutrons. Physical chemistry chunks proton and neutron systems to produce the composite particle, the nucleus. Chunking at the level of atoms and molecules gives us the continuum fluid representation. Hofstadter describes the relations among various levels of chunking:

> Although there is always some "leakage" between the levels of science, so that a chemist cannot afford to ignore lower level physics totally, or a biologist to ignore chemistry totally, there is almost no leakage from one level to a distant level. That is why people can have an intuitive understanding of other people without necessarily understanding the quark model, the structure of the nuclei, the nature of electron orbits, the chemical bond, the structure of proteins, the organelles in a cell, the methods of intercellular communication, the physiology of the various organs within the human body, or the complex interactions among organs. All that a person needs is a chunked model of how the highest level acts; and as we all know, such models are very realistic and successful.

A corollary is that chunked models no longer have the ability to predict exactly.

> In short, in using chunked high level models, we sacrifice determinism for simplicity. . . . A chunked model defines a "space" within which behavior is expected to fall, and specifies probabilities of its falling in different parts of that space.

In a complex reactive flow, it is not possible to resolve all aspects of the microscopic particle interactions using a continuum approximation. It is, however, possible to include some of the macroscopic consequences of atomic and molecular phenomena in a fluid model. Chemical reactions, interspecies molecular diffusion, thermal conductivity, temperature-dependent enthalpies and equations of state are all examples of macroscopic models of microscopic processes that result from chunking the microscopic physics.

1–4. The Hierarchy of Levels of Simulation

In this book we are not concerned with elementary particles, but with a more macroscopic view of reactive media composed of molecules and atoms. The interactions of particles at this level result in the processes we want to simulate. Table 1.1 lists the hierarchy of mathematical models used to describe the behavior of systems involving many particles and interactions. Discussions of the derivations of these various approaches can be found in a number of texts (for example, Hirschfelder, Curtiss, and Bird [1954] and Bird [1994]). At the most basic level, these techniques provide very fundamental solutions of the Schrödinger equation describing accurate quantum mechanical interactions of particles, such as might lead to quantum molecular dynamics methods. More general approximations

Table 1.1. Levels of Models of Manybody Interactions

Equation	Solution Method
Schrödinger's equation	Direct solution, density functional theory, (prescribed interparticle forces)
Newton's law $f = ma$	Molecular dynamics (particle-based, prescribed interparticle forces)
Liouville equation equation for distribution function, $F(\mathbf{x}_i, \mathbf{v}_i, t), \quad i = 1, N_p$	Monte Carlo methods (statistical, particle-based methods) Direct simulation Monte Carlo
Boltzmann equation $F(\mathbf{x}, \mathbf{v}, t)$ binary collisions (low density) good for gases	Direct solution
Navier-Stokes equation $\rho(\mathbf{x}, t), \quad \mathbf{u}(\mathbf{x}, t)$ short mean free path	Direct solution: finite differences, finite volumes, spectral methods . . . (continuum flow methods)

replace individual particles by continuum fluid elements, as in the Navier-Stokes equations. In between these extremes, there are several levels of statistical and particle-based methods that can be necessary for accurate treatment of some reactive-flow problems.

Molecular dynamics (whether quantum mechanical or classical) is one of the more fundamental levels of this hierarchy. The interactions among the particles may be represented by as basic an interaction as Newton's law in classical representations, or by extremely complex quantum mechanical potentials. The Liouville equation is the fundamental equation of statistical mechanics that describes the distribution function of a gas as a function of the $6N_p$-dimensional phase space of N_p particles (Hirschfelder et al. 1954; Goldstein 1982). Monte Carlo approaches and the Boltzmann equation are both derived from the Liouville equation. Monte Carlo methods exploit the statistical nature of multiple collisions in physical systems and have often been used to describe microscopic systems. When particle densities are high enough that the system of particles can be considered as a continuum, the Navier-Stokes equations are generally used to describe the fluid. There are also various subsets or reduced forms of the reactive Navier-Stokes equations that are commonly used today. These are models that include averages of the behavior of the small continuum scales (for example, to describe turbulent flows, Chapter 12), averages of chemical reactions (to "reduce" the chemical models, Chapter 5), or averages over radiative transport processes (Chapter 13).

Some of the information in Table 1.1 is recast into quantitative form in Figure 1.1, which shows the physical regimes of validity of different types of reactive-flow representations. The regimes of validity are shown in this figure as functions of two important parameters, a characteristic length scale of interest in the system L, and the mean molecular spacing Δ, expressed as the cube root of the inverse of the fluid density. The vertical axis is L/d, a measure of the size of the region of interest, where d is the molecular diameter. The

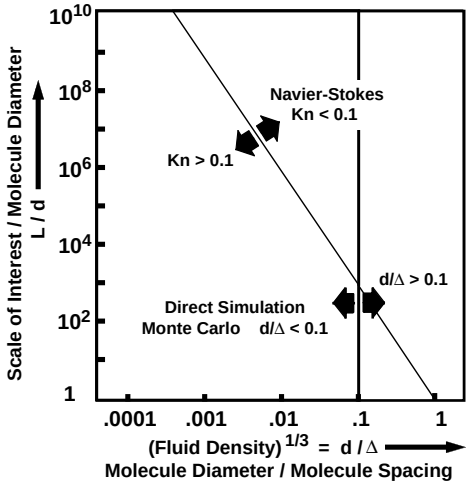

Figure 1.1. Regimes of validity of direct simulation Monte Carlo and Navier-Stokes equations, as a function of the characteristic length scale and mean molecular spacing of a system. In principle, molecular dynamics is valid throughout the entire domain.

horizontal axis shows the dilution of the fluid measured in units of the molecular diameter d divided by the mean spacing of the particles $\Delta \equiv N^{-1/3}$, where N is the number density. As the mean spacing between molecules decreases, the density, $(d/\Delta)^3$, increases. Expressed in this way, the density has a maximum value, at the right side of the figure, of about unity when the molecules are closely packed and the fluid is least dilute.

When the ratio of the mean molecular diameter, d, to the molecular spacing, Δ, is small, so that $d/\Delta \ll 1$ (for example, $d/\Delta < 0.1$), the fluid becomes *dilute*. This regime, which is on the left of the vertical line in the figure, is one in which the statistically based particle method, direct simulation Monte Carlo (DSMC) is an appropriate model (Bird 1994). DSMC is based on the same basic approximations as the Boltzmann equation, but unlike the Boltzmann equation, its regime of validity may be extended to systems where complicated chemistry and three-body collisions occur.

The *Knudsen number*, *Kn*, is another quantity that is useful in characterizing the regimes of a fluid. This is defined as $Kn \equiv \lambda/L$. Here, L is a characteristic scale length of the system, and λ is the *mean free path*, $\lambda \approx 0.1/Nd^2$, the average distance traveled by a typical molecule between collisions. When λ is small compared to L, and Kn is low enough, the medium behaves as a continuous fluid in which properties such as density, velocity, and energy are well defined at each point. In the collision-dominated regime, where $Kn < 0.1$, the Navier-Stokes model is generally valid.

Because of the different criteria for validity of the Navier-Stokes and DSMC models, both methods can be used in the triangular domain in the upper part of Figure 1.1 where $d/\Delta < 0.1$ and $Kn < 0.1$. When the diagonal line $Kn = 0.1$ is crossed from left to right, the Navier-Stokes equations become valid and are preferred to the DSMC model because of computational efficiency. Thus, this dividing line is usually the practical condition for applicability of DSMC. DSMC is used extensively for high-speed atmospheric reentry problems, where the gas is very dilute and often highly reactive.

Because molecular dynamics is based on a relatively fundamental model, it is valid in principle throughout the entire range of parameters shown. There are no *physical* reasons why it cannot be used for all ranges of densities and system sizes. However, the

computations are very expensive as the number of particles becomes large. In the small triangular regime in the lower right of the figure, neither the Navier-Stokes nor the DSMC model is valid. In this parameter regime, molecular dynamics is, therefore, the preferred model.

This book focuses on finite-volume methods for solving continuum reactive-flow problems. In this approach, time is divided into discrete intervals – *timesteps* – and space into discrete intervals – *computational cells* that define the *spatial grid* or *mesh*. Large sets of discrete variables are defined on the computational cells to approximate fluid variables such as density and velocity. This process puts the equations in a form suitable for numerical computation. We expect the corresponding numerical solutions to converge and become better representations of the continuous fluid variables as the size of the cells and timesteps becomes smaller and smaller. A continuum fluid simulation with cells smaller than a mean free path is subject to problems of physical interpretation even if the model does converge mathematically. Problems that arise due to limits on the attainable resolution are discussed in many parts of this book, but especially in Chapter 6.

Even if practical computational restrictions were removed and arbitrarily good resolution were possible, the continuous variables would still have to be represented in a computer by a discrete set of distinct real numbers with finite numerical precision. It is amusing to note that fluid equations were invented in the first place to simplify the discrete equations of individual particle dynamics. Now we find ourselves reformulating the continuum problem so that we can use digital computers to solve the equations for finite volumes of material. Nevertheless, the continuum set of equations is considerably smaller and simpler to solve than the original equations of particle dynamics.

1–5. The Growth of Computational Capability

Fifteen years ago, when the first edition of this book was written, a two-dimensional computation with 10^6 computational cells was considered very large. Steady-state approximations were the best that could be done for many systems. Today, three-dimensional computations with true dynamics have been performed with more than 10^9 cells. Complex, time-dependent simulations, that were considered an esoteric art confined to a few laboratories with large computers, can now be readily solved by most scientists and engineers on their desktop workstations. All of this reflects continuing exponential advances in computer memory and computational speed.

There have been corresponding changes in our expectations for computing reacting flows. One result of the general increase in computational resources is that proportionately fewer users are trying to develop their own numerical models. They are, instead, using complex, difficult-to-understand simulation programs that were initially written by others. One objective of this book, then, is to explain how to evaluate, use, and interpret the widespread and rapidly growing computational technology available for solving reactive-flow problems.

Figure 1.2 qualitatively illustrates these advances in computer speed and memory as a function of year (based on updating a lecture by Worlton [1988]). The essentially straight line increase of overall performance on the semilog scale means that computer power

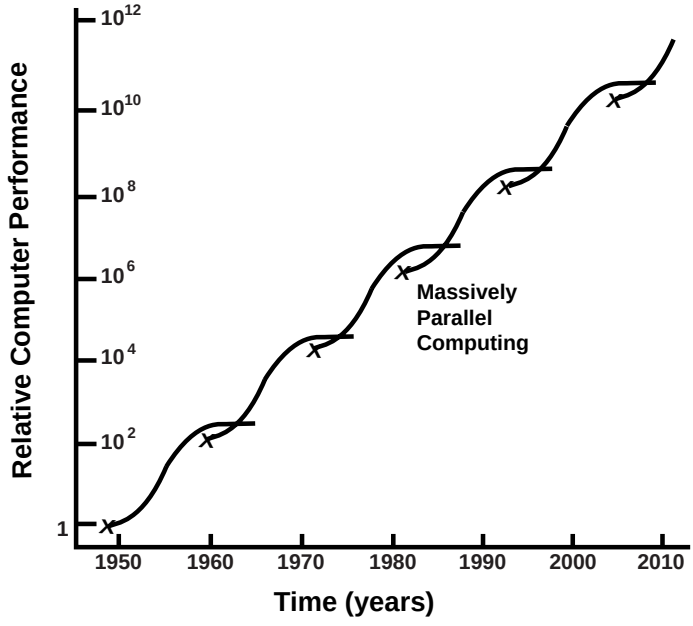

Figure 1.2. Schematic showing the exponential increase of computer power (speed and memory) as a function of time. The crosses indicate the introduction of a major technological breakthrough.

and memory are scaling exponentially. Projections based on current understanding of technology are that this rate can hold for at least another ten years. The figure shows that the exponential performance increase is really composed of a series of piecewise logistic curves, each representing the introduction of a new technology. The result of adding all of the curves is sustained exponential growth. For example, early breakthroughs have included introducing transistors to replace vacuum tubes and semiconductor memory to replace magnetic cores. More recently, we have changed from scalar to vector architectures, and from serial to parallel computing. Such a curve is typical of the growth of an enabling technology, such as high-performance computing. The time-dependent improvement of each component technology is necessarily short term, and saturates at some point. The leveling occurs because the particular technology that allowed the growth becomes too expensive and time-consuming to improve. One obvious feature of this curve is that to continue the growth, and not stagnate, new technologies must regularly be discovered.

Along with the development of high-end computing, there have been the corresponding improvements in personal computers and desktop workstations. As hardware and software become more sophisticated, computing improves across the board. Currently, most parallel supercomputers have about the same speed per processor because they are based on the same or similar chips. The performance increases are driven by microprocessor technology rather than research and development aimed at supercomputer architectures. The current design philosophy tends to use the same basic components (chips) for both supercomputers and powerful workstations. This philosophy may slow the overall pace of computer development, since the high-end systems are less and less the drivers of new

technology. Alternately, it could speed the pace as there is broad-based public demand for faster desktop computing. This is a curious interplay that has practical consequences for scientific computing.

The differences among high-end computers are in their interprocessor communications, memory structures, and architectures. The memory may be globally shared or distributed among the processors. Interprocessor communications may or may not scale linearly as a system expands from a few processors to many processors, and various problems can arise in sending data among processors. At another level, the different architectures cause problems in moving computer programs from one type of machine to another (the portability problem). The current goal is to obtain computational speeds of many teraflops (10^{12} floating-point operations per second), whereas computers delivering many gigaflops (billions of floating-point operations per second) are becoming common.

New advances in algorithms and computer architectures have made a significant contribution to computing reacting flows. Progress has also come through the straightforward application of various existing algorithms as well as from new procedures that combine the standard algorithms with specific features of the new architectures. Future advances could also come from simultaneously combining different kinds of computers, each of which is best suited for a different type of operation, an approach called heterogeneous computing. Another approach uses different sets of processors on the same computer to perform different kinds of operations.

1–6. The Tyranny of Numbers

A detailed numerical simulation model is a program that is executed, or "run," on a computer. The final accuracy and detail we can expect from a numerical simulation of a reactive flow depends on the interplay of a number of factors, including the availability of high-speed computers, specialized numerical algorithms, and fast visualization of the output. The simulations we are concerned with "integrate," or "advance," the approximate time-evolution equations of the model from one time t to another time $t + \Delta t$, where Δt is the *timestep* and is generally smaller than the shortest characteristic times we need to resolve in the calculation. The advancing simulation thus defines the changing state of the system at a sequence of discrete times. The usual assumption is that the state of the system at any time during a timestep can be inferred by interpolating between the state of the system at the beginning and at the end of the timestep.

Typically, hundreds of thousands to millions of numbers are needed to specify the state of a system at any particular time. Consider a detonation propagating in a gas-phase reactive medium. If the problem is two-dimensional, roughly 200×200 discrete points in space are required to give about 1 percent spatial resolution of the flow field and of the chemical species present. If a detailed chemical rate scheme for a diluted hydrogen-oxygen mixture is used, approximately ten species have to be considered in addition to the total fluid density, momentum, and energy density variables. Thus, a minimum of 560,000 numbers are required to specify any state of this modest system at a given time. Realistic simulations are regularly performed for 10^7 variables at a few seconds per timestep, which gives thousands of timesteps per hour of computer time. A major practical problem is how to cope with and effectively interpret so many numbers. We cannot afford

to store all the data from every timestep, nor is it generally useful to do this. Even if the cost of computer memory continues to drop, the time needed to store, compute, and transmit all of these numbers can make a simulation impossibly large and cumbersome.

The tyranny of numbers that plagues most detailed reactive-flow simulations also hampers diagnosis of the computed physical results. To look at the actual numbers associated with just one of the many variables describing a single timestep entails printing out approximately 40,000 numbers, or about forty single-spaced pages of output. If a comparison solution were actually printed out at the same time, eighty pages would be needed. The graphics and diagnostics needed to address this tyranny of numbers effectively can be as time consuming and expensive to develop, apply, and use, as the simulation itself.

In addition to producing large amounts of data, detailed numerical simulations usually require large amounts of computer time. For this reason, simulations are run in segments of generally a few thousand timesteps. Thus, software must be provided to "dump" and save the information describing a particular state of the system at selected timesteps. The calculation can then be restarted from this data at a later time with the option of changing the parameters or the diagnostics.

1–7. A Bridge between Theory and Experiment

Detailed numerical simulation is often the only way to produce general solutions of a complex mathematical model. It is a tool for studying physical systems that bridges theoretical analysis and laboratory experiments. As such, detailed simulations have some of the advantages and the disadvantages of both. This book gives practical procedures for implementing and interpreting chemically reactive-flow models on a computer. It also discusses many numerical algorithms for solving the model equations.

Simulations as Computer Experiments

A detailed computer simulation is not an analytic theory; it does not give equations relating physical variables to each other and to the parameters of the problem. Each simulation is a unique computer experiment that has been performed with one set of geometric, physical, initial, and boundary conditions. The simulation can tell us about something new and unexpected when the model is complete enough, much as a laboratory experiment can teach us something new about the physical environment.

Simulations and experiments contain similar types of errors. In simulations, some of the errors are caused by bugs in the program and are analogous to experimental errors such as leaks or undetected sources of external energy. Calibration errors in an experiment are similar to invalid input constants, parameters, or submodels in a detailed simulation. If the calibrations are incorrect, an experimental apparatus may still be working well. The results, or the interpretation of the data, will be wrong. By the same reasoning, if the chosen values for the controlling chemical rate constants in a simulation are incorrect, the results of the simulation are wrong even though the simulation may be quantitatively accurate for the problem actually specified.

For example, consider an experiment in which streams of hydrogen and oxygen molecules leave a container, mix, and react. Various reactions dominate, depending on the

pressure and density, or on the concentration of impurities or additives present, and so on. To give physically accurate results, a simulation must include a correct chemical mechanism to describe the actual behavior in a natural way. It is usually difficult to know what is missing or what is incorrect when a simulation does not agree with an experiment.

Whereas simulation diagnostics are possible sources of error, the errors associated with experimental diagnostics can also cause problems. Simulation diagnostics can be performed without interfering in the basic computations, but laboratory measurements may perturb the experiment itself. Experimental probes can change the local flow, provide sites for unwanted surface reactions, and absorb heat from the medium. This problem does not exist in the computer experiment.

Both simulations and laboratory experiments benefit greatly from focusing on specific mechanisms and interactions. For example, geometric complications, such as multidimensional effects and wall boundary effects, make both simulations and experiments more difficult. Much can be learned about fundamental interactions by idealizing and simplifying the problem as much as possible. The insight to construct systems for computational study that accomplish this simplification requires a different set of skills from those required for mathematical analysis.

Simulations as Extensions of Theory

Although a simulation may not provide the types of analytic relationships that a theory gives, it provides a similar flexibility. This flexibility is its ability to evaluate the importance of a physical effect by turning the effect on or off, changing its strength, or changing its functional form. This straightforward way of isolating interactions is also an important advantage over experiments. In fact, an experiment is not always a better probe of our physical environment than is a simulation.

Simulations may be used to test the range of validity of theoretical approximations. When a linear theory breaks down, the manner of breakdown can be studied by simulations. Fluid dynamic simulations have been used to study the nonlinear evolution of the Kelvin-Helmholtz and Rayleigh-Taylor instabilities. Theories of transition to turbulence, turbulent boundary layers, and chaotic nonlinear dynamics are other examples where simulations have been used to test and extend theory.

The converse is also true: theory plays a crucial role in validating a numerical model. Exact comparisons with closed-form solutions provide the most valuable benchmarks to verify the computational model. By turning off the terms in the simulation that the theoretical solution does not include, the accuracy and failure modes of parts of the computer model can be evaluated before the program is used to study a more physically complex configuration in which similar errors may go undetected.

Simulation Can Bridge the Gap between Theory and Experiment

Because results obtained from a detailed model may be more comprehensive than those from an analytic theory, detailed models can be used to bridge the gap between theory and experiment. In particular, an effective bootstrap approach to solving problems is to use detailed simulation models to calibrate phenomenological models of specific processes and interactions. These phenomenological models can then be used in the detailed model

to extend its range of validity or its effective resolution. Proposed physical laws can be tested by including the major processes they describe in a simulation and then comparing the results of the simulations and experiments. The use of detailed simulation models to calibrate quantitative understanding of the controlling physical processes is perhaps their most important and fundamental use.

1–8. Themes of This Book

Several interrelated themes recur throughout this book. These themes provide guidelines for developing, carrying out, and interpreting reactive-flow simulations. They present points of view that should be helpful and relate some useful rules of thumb that we have developed after doing many simulations.

Choosing the Type and Level of Simulation

We have already differentiated between modeling based on phenomenologies and empirical laws and modeling from first principles. We also introduced the idea of chunking, which helps determine the level for each component process in the overall simulation. The optimal combination of modeling approaches depends as much on the resources available and the type of answer required as on the parameters of the system being simulated.

Our experience has led us to conclude that reactive flows are generally unsteady, and so the methodology of numerical simulations treated in this book focuses on reproducing time-dependent behavior. We have too often found that steady-state models are unreliable in that they do not reproduce the behavior of the reactive flow: too often they give answers that are both qualitatively as well as quantitatively incorrect. Time-dependent simulations may be used to "march" to a steady state, or their results may be used to produce averages that are suitable for comparing to experimental data.

Building Modular Simulation Models

In a modular approach, the problem is divided into a number of individual physical processes. Models can be built so that each of these processes is calculated accurately and calibrated separately. The resulting algorithms are then coupled together to study the resulting composite reactive-flow mechanisms and interactions. In addition to providing a reasonable organization for attacking the overall problem, this approach allows use of the best algorithm for each aspect of the problem and provides a flexible framework for attacking other problems.

Evaluating Numerical Methods for Accuracy and Efficiency

Throughout this text, we will be evaluating numerical methods with respect to what they can and cannot do in reactive-flow calculations. We try to explain their strong and weak points, emphasizing their accuracy, efficiency, ease of use, and flexibility. We try to introduce more advanced methods in many places and point out some areas to watch for important computational developments.

When the objective is to solve a particular kind of reactive-flow problem, the best methods to use are those which have been extensively tested and debugged. It is crucial

to compare simplified analytic solutions with the output of the simulations when developing numerical simulation models. This check should be done with each process as it is programmed and with combinations of processes whenever possible. It is particularly important to do these tests when developing a new model, and to repeat them after any major changes have been made. Throughout the book, we will return to this theme because success with numerical simulation of reactive flow is as much governed by the reliability of your results as by the results themselves.

Trade-offs

There are trade-offs in every step of the process: in selecting the problem, developing the model, developing the numerical algorithms, building computer programs, and so forth. It is extremely useful to be aware of these and how they affect the solution. Such considerations are a persistent theme from Chapter 3 to the end of the book.

Computational Rules of Thumb

A number of useful "rules of thumb" for simulating reactive flows are given throughout the book. They have evolved from common sense and working through the trade-offs required to find optimum algorithms for each of the relevant physical processes and then for coupling them together.

REFERENCES

Bird, G.A. 1994. *Molecular gas dynamics and the direct simulation of gas flows*. Oxford, England: Oxford University Press.

Goldstein, H. 1982. *Classical mechanics*. 2d ed. Reading, Mass: Addison-Wesley.

Hirschfelder, J.O., C.F. Curtiss, and R.B. Bird. 1954. *Molecular theory of gases and liquids*. New York: Wiley (corrected with notes added, 1964).

Hofstadter, D.R. 1979. *Gödel, Escher, Bach: An eternal golden braid*. New York: Basic Books.

Worlton, J. 1988. *Some patterns of technological change in high-performance computers*. In *Proceedings of supercomputing '88*. Washington, D.C.: IEEE Computing Society Press.